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Starting from an exact lower bound on the imaginary-time propagator, we present a Path-Integral Quantum Monte Carlo method that can handle singular attractive potentials. We illustrate the basic ideas of this Quantum Monte Carlo algorithm by simulating the ground state of hydrogen and helium.

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I. INTRODUCTION

Quantum Monte Carlo (QMC) simulation is a powerful method for computing the ground state and non-zero temperature properties of quantum many-body systems [1,2]. There are two fundamental problems that limit the application of these methods. The first and most important is the minus-sign problem on which we have nothing to say in this paper, see however [3,4]. The second problem arises if one would like to simulate systems with attractive singular potentials, the Coulomb interaction being the prime example. The purpose of this paper is to present an approach that solves the latter problem, in a form that fits rather naturally in the standard Path Integral QMC (PIQMC) approach and leaves a lot of room for further systematic improvements.

Let us first recapitulate the basic steps of the procedure to set up a PIQMC simulation. Writing K and V for the kinetic and potential energy respectively the first step is to approximate the imaginary-time propagator by a product of short-time imaginary-time propagators. The standard approach is to invoke the Trotter-Suzuki formula [5,6]

$$e^{-\beta(K+V)} = \lim_{m\to\infty} \left(e^{-\beta K/m} e^{-\beta V/m)}\right)^m, \tag{1}$$

to construct a sequence of systematic approximations Z_m to the partition function Z [6,7]:

$$Z = \mathbf{Tr}\exp(-\beta H) = \lim_{m\to\infty} Z_m \tag{2}$$

$$Z_m = \int dr_1 \cdots dr_m \prod_{n=1}^{m} \langle r_n|e^{-\beta K/m}|r_{n+1}\rangle e^{-\beta V(r_{n+1})/m}, \tag{3}$$

where $r_{m+1} = r_1$ and use has been made of the fact that the potential energy is diagonal in the coordinate representation. Taking the limit $m \to \infty$, (3) yields the Feynman path integral [9] for a system with Hamiltonian $H = K + V$. Expression (3) is the starting point for PIQMC simulation.

In the case the attractive Coulomb interaction, it is easy to see why the standard PIQMC approach fails. Let us take the hydrogen atom as an example. The Hamiltonian reads

$$H = -\frac{\hbar^2}{2M}\nabla^2 - \frac{q^2}{r}, \tag{4}$$

where q denotes the charge of the electron and $M = m_e/(1 + m_e/m_p)$, m_e (m_p) being the mass of the electron (proton). Replacing the imaginary-time free-particle propagator in (3) by its explicit, exact expression

$$\langle r|e^{-\beta K/m}|r'\rangle = \left(\frac{mM}{2\pi\beta\hbar^2}\right)^{3/2} \exp\left(-\frac{mM|x-x'|^2}{2\beta\hbar^2}\right), \tag{5}$$

we obtain

$$Z_m = \left(\frac{mM}{2\pi\beta\hbar^2}\right)^{3m/2} \int dr_1 \cdots dr_m \exp\left[-\frac{mM}{2\beta\hbar^2}\sum_{n=1}^{m}(r_n - r_{n+1})^2\right] \exp\left[+\frac{\beta q^2}{m}\sum_{n=1}^{m}\frac{1}{r_n}\right]. \tag{6}$$

PIQMC calculates ratio of integrals such as (6) by using a Monte Carlo procedure to generate the coordinates $\{r_1, \ldots, r_m\}$. The integrand in (6) serves as the weight for the importance sampling process. As the latter tends to

maximize the integrand, it is clear that because of the factors $\exp\left(+\beta q^2 m^{-1} r_n^{-1}\right)$, the points $\{r_1,\ldots,r_m\}$ will, after a few steps, end up very close to the origin. In the case of a singular, attractive potential importance sampling based on (6) fails. Using instead of the simplest Trotter-Suzuki formula (1) a more sophisticated one [8] only makes things worse because these hybrid product formulae contain derivatives of the potential with respect to the coordinates.

The problem encountered in setting up a PIQMC scheme for models with a singular, attractive potential is just a signature of the fundamental difficulties that arise when one tries to define the Feynman path integral for the hydrogen atom [10]. The formal solution to this problem is known [10,11]. It is rather complicated and not easy to incorporate in a PIQMC simulation.

In spirit the method proposed in this paper is similar to the one used to solve the hydrogen path integral: Use the quantum fluctuations to smear out the singularity of the potential. Mathematically we implement this idea by applying Jensen's inequality to the propagator [12]. Applications of the Feynman path-integral formalism are often based on a combination of Jensen's inequality and a variational approach [9,10] so it is not a surprise that similar tricks may work for PIQMC as well.

The paper is organized as follows. In Section 2 we give a simple derivation of an exact lower bound on the imaginary-time propagator. This inequality naturally defines a sequence of systematic approximations $\hat{Z}_m$ to the partition function. Although each $\hat{Z}_m$ looks very similar to Z_m, the former can be used for PIQMC with attractive, singular potentials. For pedagogical reasons, in Section 3 we illustrate the approach by presenting an analytical treatment of the harmonic oscillator. In Section 4 we give the explicit form of the approximate propagator for the attractive Coulomb potential and present PIQMC results for the ground state of the hydrogen and helium atom.

II. LOWER BOUND ON THE PROPAGATOR

Consider a system with Hamiltonian $H = K + V$ and a complete set of states $\{|x\rangle\}$ that diagonalizes the hermitian operator V. In the case that V contains a singular attractive part we replace $V = \lim_{\epsilon\to 0} V_\epsilon$ by a regular $V_\epsilon(x) > -\infty$ and take the limit $\epsilon \to 0$ at the end of the calculation. Using the Trotter-Suzuki formula we can write

$$\begin{aligned}
\langle x|e^{-\tau(K+V_\epsilon)}|x'\rangle &= \lim_{m\to\infty}\langle x|\left(e^{-\tau K/m}e^{-\tau V_\epsilon/m}\right)^m|x'\rangle, &(7)\\
&= \lim_{m\to\infty}\int dx_1\cdots dx_n\prod_{i=1}^m\langle x_i|e^{-\tau K/m}|x_{i+1}\rangle e^{-\tau V_\epsilon(x_i)/m}, &(8)\\
&= \lim_{m\to\infty}\frac{\int dx_1\cdots dx_n\prod_{i=1}^m\langle x_i|e^{-\tau K/m}|x_{i+1}\rangle e^{-\tau V_\epsilon(x_i)/m}}{\int dx_1\cdots dx_n\prod_{i=1}^m\langle x_i|e^{-\tau K/m}|x_{i+1}\rangle}\int dx_1\cdots dx_n\prod_{i=1}^m\langle x_i|e^{-\tau K/m}|x_{i+1}\rangle &(9)
\end{aligned}$$

If $\langle x|e^{-\tau K}|x'\rangle \geq 0$ for all τ, x and x', the function

$$\rho(\{x_i\}) = \prod_{i=1}^m\langle x_i|e^{-\tau K/m}|x_{i+1}\rangle\Big/\int dx_1\cdots dx_n\prod_{i=1}^m\langle x_i|e^{-\tau K/m}|x_{i+1}\rangle, \tag{10}$$

is a proper probability density. Clearly (10) is of the form $\int dx_1\cdots dx_n\rho(\{x_i\})f(\{x_i\})$ so that we can apply Jensen's inequality

$$\int dx_1\cdots dx_n\rho(\{x_i\})e^{g(\{x_i\})} \geq \exp\left(\int dx_1\cdots dx_n\rho(\{x_i\})g(\{x_i\})\right), \tag{11}$$

and obtain

$$\begin{aligned}
\langle x|e^{-\tau(K+V_\epsilon)}|x'\rangle &\geq \langle x|e^{-\tau K}|x'\rangle\lim_{m\to\infty}\exp\left(-\frac{\tau}{m}\sum_{i=1}^m\int dx_1\cdots dx_m\frac{V_\epsilon(x_i)\prod_{n=1}^m\langle x_n|e^{\tau K/m}|x_{n+1}\rangle}{\langle x|e^{-\tau K}|x'\rangle}\right), &(12)\\
&\geq \langle x|e^{-\tau K}|x'\rangle\lim_{m\to\infty}\exp\left(-\frac{\tau}{m}\sum_{i=1}^m\int dx_i\frac{\langle x|e^{\tau K/m}|x_i\rangle V_\epsilon(x_i)\langle x_i|e^{\tau K/m}|x'\rangle}{\langle x|e^{-\tau K}|x'\rangle}\right). &(13)
\end{aligned}$$

For $m\to\infty$, the sum over n can be replaced by an integral over imaginary time. Finally we let $\epsilon\to 0$ and obtain [12]

$$\langle x|e^{-\tau(K+V)}|x'\rangle \;\geq\; \langle x|e^{-\tau K}|x'\rangle \exp\left\{-\int_0^\tau du \frac{\langle x|e^{-uK}Ve^{-(\tau-u)K}|x'\rangle}{\langle x|e^{-\tau K}|x'\rangle}\right\}. \tag{14}$$

Note that l.h.s of (14) reduces to the standard, symmetrized Trotter-Suzuki formula approximation [13,14] if we replace the integral over u by a two-point trapezium-rule approximation. This replacement also changes the direction of inequality as can been seen directly from the upperbound [12]

$$\langle x|e^{-\tau(K+V)}|x'\rangle \;\leq\; \langle x|e^{-\tau K}|x'\rangle \exp\left\{-\int_0^\tau du \ln\left(\frac{\langle x|e^{-uK}e^{-\tau V}e^{-(\tau-u)K}|x'\rangle}{\langle x|e^{-\tau K}|x'\rangle}\right)\right\} \leq \langle x|e^{-\tau K}|x'\rangle e^{-\tau V(x)}. \tag{15}$$

Expression (14) can be used to define a new type of approximant to the partition function namely

$$\hat{Z}_m = \left(\frac{M}{2\pi\tau\hbar^2}\right)^{3m/2} \int dr_1 \ldots dr_m \prod_{n=1}^{m} \exp\left[-\frac{M}{2\tau\hbar^2}(r_n - r_{n+1})^2 - \int_0^\tau du \frac{\langle r_n|e^{-uK}Ve^{-(\tau-u)K}|r_{n+1}\rangle}{\langle r_n|e^{-\tau K}|r_{n+1}\rangle}\right]. \tag{16}$$

where $\tau = \beta/m$. The simplest approximant $\hat{Z}_1$ corresponds to the Feynman's variational approximation to the full Feynman path integral [9,10]. The main difference between (3) and (16) is that the bare potential $e^{-\tau V(x)}$ is replaced by an effective potential that is obtained by convoluting the bare potential and free-particle propagators e^{-uK} and $e^{-(\tau-u)K}$. Convolution smears out singularities. As we show below, in the case of the attractive Coulomb interaction expression (14) is finite, for any choice of x and x'. For the approximants $\hat{Z}_m$ to be useful in PIQMC, it is necessary that the integral over u can be done efficiently. In the next two sections we show how this can be done.

III. ILLUSTRATIVE EXAMPLE

It is instructive to have at least one example for which the details can be worked out analytically, without actually using PIQMC. Not surprisingly this program can be carried out for the harmonic oscillator. For notational convenience we will consider the one-dimensional model Hamiltonian $H = K + V$, with $K = -(\hbar^2/2M)d^2/dx^2$ and $V = M\omega^2x^2$. Calculating the matrix element $\langle x|e^{-uK}Ve^{-(\tau-u)K}|x'\rangle$ in (16) is a straightforward excercise in perfoming Gaussian integrals [15]. We obtain

$$\hat{Z}_m = \left(\frac{mM}{2\pi\beta\hbar^2}\right)^{m/2} \int dx_1 \ldots dx_m \prod_{n=1}^{m} \exp\left[-\frac{mM}{2\beta\hbar^2}(x_n - x_{n+1})^2 - \frac{\beta M\omega^2}{6m}(x_n^2 + x_{n+1}^2 + x_n x_{n+1} + \frac{\beta\hbar^2}{2mM})\right]. \tag{17}$$

The integrand in (17) is a quadratic form and can be diagonalized by a Fourier transformation with respect to the index n. Evaluation of the resulting Gaussian integrals yields

$$\hat{Z}_m = 2^{-m/2} \exp\left(-\frac{\beta^2\hbar^2\omega^2}{12m}\right) \prod_{n=0}^{m-1} \left[1 + \frac{\beta^2\hbar^2\omega^2}{3m} - \left(1 - \frac{\beta^2\hbar^2\omega^2}{6m}\right)\cos\left(\frac{2\pi n}{m}\right)\right]^{-1/2}. \tag{18}$$

Taking the partial derivative of $-\ln\hat{Z}_m$ with respect to β gives the corresponding approximation to the energy:

$$\hat{E}_m = \frac{\beta\hbar^2\omega^2}{6m}\left[1 + \sum_{n=0}^{m-1} \frac{2 + \cos(2\pi n/m)}{1 - \cos(2\pi n/m) + \beta^2\hbar^2\omega^2\,(2 + \cos(2\pi n/m))/6m}\right]. \tag{19}$$

For comparison, if we use of the standard Trotter-Suzuki formula we obtain [7]

$$E_m = \frac{\beta\hbar^2\omega^2}{2m^2} \sum_{n=0}^{m-1} \frac{1}{1 - \cos(2\pi n/m) + \beta^2\hbar^2\omega^2/2m^2} \tag{20}$$

In Table 1 we present numerical results obtained from (19) and (20) and compare with the exact value of the energy $E = (\hbar\omega/2)\coth(\beta\hbar\omega/2))$. Note that the average of the two approximations, i.e. $(\hat{E}_m + E_m)/2$, is remarkably close to the exact value E, an observation for which we have no mathematical justification at this time.

TABLE I. Numerical results for the exact energy of the harmonic oscillator (E), and approximations based on (19) ($\hat{E}_m$) and (20) (E_m). We use units such that $\hbar\omega = 1$ and β is dimensionless.

β	m	E_m	E	$\hat{E}_m$
1	1	1.00000	1.08198	1.16668
	10	1.08101	1.08198	1.08292
	50	1.08194	1.08198	1.08202
	100	1.08197	1.08198	1.08199
	500	1.08198	1.08198	1.08198
5	1	0.20000	0.50678	1.03333
	10	0.49199	0.50678	0.51938
	50	0.50617	0.50678	0.50694
	100	0.50678	0.50678	0.50679
	500	0.50678	0.50678	0.50679
10	1	0.10000	0.50005	1.76667
	10	0.44273	0.50005	0.54316
	50	0.49757	0.50005	0.50234
	100	0.49942	0.50005	0.50064
	500	0.50002	0.50005	0.50007

IV. ATTRACTIVE COULOMB POTENTIAL

As a second example we will consider a neutral system consisting of two electrons with opposite spin and a nucleus. The Hamiltonian reads [16,17]

$$H = -\frac{\hbar^2}{2M_1}\nabla_1^2 - \frac{\hbar^2}{2M_2}\nabla_2^2 - \frac{q^2}{|r_1|} - \frac{q^2}{|r_2|} + \frac{2q^2}{|r_1 - r_2|}, \tag{21}$$

where the vectors r_1 and r_2 describe the position of the two electrons, with the nucleus placed in the origin. It is convenient to introduce the notation $K_i = -D_i\nabla_i^2$, $D_i = \hbar^2/2M_i$, $V_i = V(r_i)$, $V_{12} = V(r_1 - r_2)$, and $V(r) = q^2/|r|$, for $i = 1, 2$. Application of inequality (14) requires the evaluation of

$$\begin{aligned} I(r_1, r_2, r_1', r_2') &= -\frac{\int_0^\tau du \langle r_1 r_2|e^{-u(K_1+K_2)}(V_1 + V_2 - 2V_{12})e^{-(\tau-u)(K_1+K_2)}|r_1' r_2'\rangle}{\langle r_1 r_2|e^{-\beta(K_1+K_2)}|r_1' r_2'\rangle} \\ &= -\frac{\int_0^\tau du\langle r_1|e^{-uK_1}V_1 e^{-(\tau-u)K_1}|r_1'\rangle}{\langle r_1|e^{-\tau K_1)}|r_1'\rangle} - \frac{\int_0^\tau du\langle r_2|e^{-uK_2}V_2 e^{-(\tau-u)K_2}|r_2'\rangle}{\langle r_2|e^{-\tau K_2}|r_2'\rangle} \\ &\quad +2\frac{\int_0^\tau du\langle r_1 r_2|e^{-u(K_1+K_2)}V_{12}e^{-(\tau-u)(K_1+K_2)}|r_1' r_2'\rangle}{\langle r_1 r_2|e^{-\tau(K_1+K_2)}|r_1' r_2'\rangle}, \end{aligned} \tag{22}$$

where we made use of the fact that $[K_1, V_2] = [K_2, V_1] = 0$. It is sufficient to consider the last term of (22). Inserting a complete set of states for both particles we obtain

$$I_{12}(r_1, r_2, r_1', r_2') = \frac{\int_0^\tau du \int dr_1'' \int dr_2'' \langle r_1 r_2|e^{-u(K_1+K_2)}|r_1'' r_2''\rangle V(r_1'' - r_2'')\langle r_1'' r_2''|e^{-(\tau-u)(K_1+K_2)}|r_1' r_2'\rangle}{\langle r_1 r_2|e^{-\tau(K_1+K_2)}|r_1' r_2'\rangle}. \tag{23}$$

Inserting the explicit expression for the free-particle propagator (5), a straightforward manipulation of the Gaussian integrals in (23) gives

$$I_{12}(r_1, r_2, r_1', r_2', D) = \int_0^\tau du \int dr \left(\frac{\tau}{4\pi u(\tau-u)D}\right)^{3/2} V(r) \exp\left\{-\frac{[\tau r - (\tau-u)(r_1 - r_2) - u(r_1' - r_2')]^2}{4u\tau(\tau-u)D}\right\}, \tag{24}$$

where $D = D_1 + D_2$

In the case of the Coulomb potential, the integral over r can be evaluated analytically by changing to spherical coordinates. The remaining integral over u is calculated numerically. In practice, it is expedient to replace the integration over u by an integration over an angle. An expression that is adequate for numerical purposes is

$$I_{12}(r_1, r_2, r_1', r_2', D) = 2\tau q^2 \int_0^{\pi/2} d\phi \frac{\mathrm{erf}\left[(4\tau D)^{-1/2}|(r_1 - r_2)\tan\phi + (r_1' - r_2')\cot\phi|\right]}{|(r_1 - r_2)\tan\phi + (r_1' - r_2')\cot\phi|}. \tag{25}$$

It is easy to check that $I_{12}(r_1, r_2, r_1', r_2', D)$ is finite. The expressions for the first and second contributions in (22) can be obtained from (25) by putting (D_2, r_2, r_2') and (D_1, r_1, r_1') equal to zero, i.e. $I_1(r_1, r_1', D_1) = I_{12}(r_1, 0, r_1', 0, D_1)$ and $I_2(r_2, r_2', D_2) = I_{12}(0, r_2, 0, r_2', D_2)$.

For the helium atom $M = M_1 = M_2$, and the m-th approximant to the partition function reads

$$\begin{aligned} \hat{Z}_m^{He} = \left(\frac{M}{2\pi\tau\hbar^2}\right)^{3m} \int \quad & dr_1 \ldots dr_m dr_1' \ldots dr_m' \exp\left\{-\frac{M}{2\tau\hbar^2}\sum_{n=1}^m \left[(r_n - r_{n+1})^2 + (r_n' - r_{n+1}')^2\right]\right\} \\ & \times \exp\left\{\tau\sum_{n=1}^m \left[I_1(r_n, r_{n+1}, D_1) + I_2(r_n', r_{n+1}', D_1) - 2I_{12}(r_n, r_{n+1}, r_n', r_{n+1}', 2D_1)\right]\right\}, \end{aligned} \tag{26}$$

whereas in the case of the hydrogen atom we have

$$\hat{Z}_m^H = \left(\frac{M}{2\pi\tau\hbar^2}\right)^{3m/2} \int dr_1 \dots dr_m \exp\left\{-\frac{M}{2\tau\hbar^2}\sum_{n=1}^{m}(r_n - r_{n+1})^2 + \tau\sum_{n=1}^{m} I_1(r_n, r_{n+1}, D_1)\right\}, \tag{27}$$

with $\tau = \beta/m$. As the integrands in (26) and (27) are always finite, expressions (26) and (27) can be used perform PIQMC simulations.

In the path integral formalism the ground state energy is obtained by letting $\beta \to \infty$ and $\beta/m \to 0$, i.e. $E = \lim_{\beta\to\infty}\lim_{\beta/m\to 0}\hat{E}_m$. Of course, in numerical work, taking one or both these limits is impossible. In Tables 2 and 3 we present numerical results of PIQMC estimates of the ground state energy E of the hydrogen and helium atom. These results have been obtained from five statistically independent simulations of 100000 Monte Carlo steps per degree of freedom each. The systematic errors due to the discretization of the path integral are hidden in the statistical noise. The PIQMC procedure we have used is standard [1,7] except for a trick we have used to improve the efficiency of sampling the paths, details of which are given in the appendix. Although a ground state calculation pushes the PIQMC method to point of becoming rather inefficient, the numerical results are in satisfactory agreement with the known values.

V. DISCUSSION

We have show that is possible to perform PIQMC simulations for quantum systems with attractive Coulomb potentials. Instead of the conventional Trotter-Suzuki formula approach one can use (16) to construct a path integral that is free of singularities. In practice, a numerical calculation of the latter requires only minor modifications of a standard PIQMC code.

The efficiency of the PIQMC method describe above can be improved with relatively modest efforts. Instead of using the free-particle propagator K, we are free to pick any other model Hamiltonian H_0 for which the matrix elements of $e^{-\tau H_0}$ are positive and integrals involving these matrix elements are known analytically. An obvious choice would be to take for H_0 a set of harmonic oscillators. The matrix elements of $e^{-\tau H_0}$ are Gaussians and hence the conditions used to derive (14) are satisfied. If necessary the approximant $\hat{Z}_m$ can be improved further by optimization of the parameters of the oscillators. For $m = 1$ this approach is identical to the variational method proposed by Feynman and Kleinert [18–21] and independently by Giachetti and Tognetti [22,23]. Extending the PIQMC method in this direction is left for future research.

TABLE II. Path-integral Quantum Monte Carlo results for the ground state energy of the hydrogen Hamiltonian, in units of q^2/a_0 ($a_0 = \hbar^2/Mq^2$). The exact value is $E = -0.5$.

β	m	$\hat{E}_m^H$
20	400	-0.496 ($\pm$ 0.004)
20	800	-0.503 ($\pm$ 0.005)
40	800	-0.498 ($\pm$ 0.006)

TABLE III. Path-integral Quantum Monte Carlo results for the ground state energy of the helium Hamiltonian, in units of q^2/a_0. The experimental value is $E = -2.904$.

β	m	$\hat{E}_m^{He}$
10	400	-2.84 ($\pm$ 0.02)
10	800	-2.88 ($\pm$ 0.02)
10	1200	-2.92 ($\pm$ 0.03)

APPENDIX

In PIQMC the simplest mehod for sampling paths is to change one degree of freedom at each Monte Carlo step. Usually this is rather inefficient and one adds Monte Carlo moves that make global changes of the path, e.g. moves that resembles the classical motion. In this appendix we present a more sophisticated scheme which we found performed very well at very low temperature. The basic idea is to change variables such that the kinetic energy term in the path integral becomes a diagonal quadratic form, i.e.

$$\sum_{k=1}^{m} (x_k - x_{k+1})^2 = \sum_{k=2}^{m} y_k^2, \tag{28}$$

where $x_{m+1} = x_1$. After some straightforward algebra one finds that the transformation from the $\{x_i\}$ to the $\{y_i\}$ is given by

$$y_k^2 = \frac{m-k+2}{m-k+1} \left(x_k - \frac{(m-k+1)x_{k-1} + x_{m+1}}{m-k+2} \right)^2 . \tag{29}$$

The expression for x_k in terms of the $\{u_i\}$ reads

$$x_k = y_1 + \sum_{j=2}^{k} \frac{m-k+1}{m-j+1} \left(\frac{m-j+1}{m-j+2} \right)^{1/2} y_j, \quad 1 < k \leq m, \tag{30}$$

with $x_1 = y_1$. From (30) we conclude that the computational work for making a global change of the path (i.e. simultaneously changing all y_i) is linear in m, hence optimal. It is also clear that the variable y_1 plays the role of the "classical" position. The variables $y_2, \ldots, y_m$ describe the quantum fluctuations.

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